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FILE COVERS 1907 - 31 Jan 2003 VOL 138 ISS 6 FILE LAST UPDATED: 30 Jan 2003 (20030130/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L5 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

2002:803368 CAPLUS

DOCUMENT NUMBER:

138:24764

TITLE:

Copper(I) Hydride-Catalyzed Asymmetric Hydrosilylation

of Heteroaromatic Ketones

AUTHOR (S):

Lipshutz, Bruce H.; Lower, Asher; Noson, Kevin

CORPORATE SOURCE:

Department of Chemistry and Biochemistry, University of California-Santa Barbara, Santa Barbara, CA, 93106,

USA

SOURCE:

Organic Letters (2002), 4(23), 4045-4048

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER:

American Chemical Society

DOCUMENT TYPE: LANGUAGE: Journal English

OTHER SOURCE(S):

CASREACT 138:24764

GΙ

AB In situ generation of CuH ligated by Takasago's new nonracemic ligand, DTBM-SEGPHOS I (RR1 = OCH2O, Ar = 3,5-di-tert-butyl-4-methoxy), leads to an esp. reactive reagent capable of effecting asym. hydrosilylation of heteroarom. (H) ketones under very mild conditions. PMHS serves as an inexpensive source of hydride. Substrate-to-ligand ratios on the order of 2000:1 are employed. A comparison was also made with in situ generated I (R = H, R1 = OMe, Ar = 3,5-di-tert-butyl-4-methoxy, 3,5-dimethylphenyl).

IT 210169-40-7

RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(copper hydride diphosphine complex in situ generation and catalyst for asym. hydrosilylation of heteroarom. ketones)

RN 210169-40-7 CAPLUS

CN Phosphine, [(4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis[3,5-bis(1,1-dimethylethyl)-4-methoxyphenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 2002:778057 CAPLUS

DOCUMENT NUMBER:

137:294761

TITLE:

Chemical bond forming reactions using

.alpha.-halocarbonyl compounds and transmetalation

reagents.

CODEN: PIXXD2

INVENTOR (S):

Zhang, Xumu; Lei, Aiwen

PATENT ASSIGNEE(S):

The Penn State Research Foundation, USA

SOURCE:

PCT Int. Appl., 35 pp.

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.		KI	ND	DATE			A	PPLI	CATI	ON NO	Ο.	DATE					
	WO 2002079339			A	2	2002	1010		W	0 20	 02-U	S962	3	2002	0329			
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
															GB,			
															KZ,			
															NO,			
			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	ŞL,	TJ,	TM,	TN,	TR,	TT,	TZ,
															KG,			
			ΤJ,									•			•	•	•	•
		RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	CH,
			CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,
															NE,			
	US	2002	1935	43	A.	1	2002	1219		U.	5 20	02-1	0842	0 ^	20020	0329	•	
US 2002193543 A1 20021219 US 2002-108420 20020329 PRIORITY APPLN. INFO.: US 2001-280275P P 20010330																		
OTHE	OTHER SOURCE(S): CASREACT 137:294761																	
AB																		
	.alphahalocarbonyl compd. with .gtoreq.1 transmetalation reagent																	
	comprising a target compd., and forming a chem. bond to or within the							ne										
	target compd. The transmetalation reagents are formed by the addn. of a							of a										
	metal or metal catalyst to a target compd. The target compd. is the								3									
	compd. undergoing chem. bond formation. Bond formation can be carried out							ied out										
	in both intermol. or intramol. reactions. Thus, reaction of																	
	3,5-dimethylphenylboronic acid in the presence of Pd2(dba)3.CHCl3,																	
	rac	-BIN	AP,	and I	KF ir	ı di	oxane	gav	7e 9'	78 3,	, 3 ' , 5	5,51	-teti	came	thvlk	oiphe	envl.	
IT	244	261-	66-3					-		•	•	•			1	1	4 -	
	RL:	CAT	(Ca	talys	st us	se);	USES	3 (Us	ses)									
										ing .	.alph	nah	nalo	carb	onyl	comp	ds.	and
		trans	smet	alati	lon 1	reag	ents)			_	-				1	T		

Phosphine, [(4R)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[diphenyl- (9CI)

244261-66-3 CAPLUS

(CA INDEX NAME)

L5 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 2002:391724 CAPLUS

DOCUMENT NUMBER:

136:401880

TITLE:

RN

CN

Ortho substituted chiral phosphines and phosphinites and their use in asymmetric catalytic reactions

INVENTOR(S):

Zhang, Xumu

PATENT ASSIGNEE(S):

The Penn State Research Foundation, USA

SOURCE:

PCT Int. Appl., 122 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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PATENT NO.
                        KIND DATE
                                                APPLICATION NO. DATE
                               _____
                                                 -----
                                              WO 2001-US43779 20011116
                        A1 20020523
     WO 2002040491
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
              GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
              RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,
              VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
              CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
              BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                                AU 2002-16719
     AU 2002016719
                         A5
                               20020527
                                                                    20011116
                               20020912
                                                US 2001-991261
     US 2002128501
                          A1
                                                                    20011116
                                             US 2000-249537P P 20001117
PRIORITY APPLN. INFO.:
                                             US 2001-301221P P
                                                                    20010627
                                             WO 2001-US43779 W 20011116
```

OTHER SOURCE(S):

CASREACT 136:401880; MARPAT 136:401880

GI

$$Z \downarrow X \\ Z \downarrow YPT_2 \\ Z_1 \downarrow YPT'_2 \\ Z_1 \downarrow X1$$

Ι

AΒ 3,3'-Substituted chiral biaryl phosphine and phosphinite ligands, I (X, X' = independently (un)substituted alkyl, (un)substituted aryl, alkoxy, organothio, diorganoamido, alkoxycarbonyl, halo, organosilyl, diorganophosphonyl, dialkoxyphosphino; Z, Z1 = independently (un) substituted alkyl, (un) substituted aryl, alkoxy, organothio, diorganoamido, alkoxycarbonyl, halo, organosilyl, diorganophosphonyl, dialkoxyphosphino, bridging group, etc.; Z', Z'', Zl', Zl'' = independently H, (un) substituted alkyl, (un) substituted aryl, alkoxy, organothio, diorganoamido, alkoxycarbonyl, halo, organosilyl, diorganophosphonyl, dialkoxyphosphino, bridging group, etc.; Y, Y' = O, CH2, NH, S, a bond between carbon and phosphorus, etc.; T, T' = (un) substituted alkyl, (un) substituted aryl, alkoxy, etc.) and metal

complexes based on such chiral ligands useful in asym. catalysis are disclosed. The metal complexes are useful as catalysts in asym. reactions, such as, hydrogenation, hydride transfer, allylic alkylation, hydrosilylation, hydroboration, hydrovinylation, hydroformylation, olefin metathesis, hydrocarboxylation, isomerization, cyclopropanation, Diels-Alder reaction, Heck reaction, isomerization, Aldol reaction, Michael addn., epoxidn., Kinetic resoln. and [m+n] cycloaddn. The metal complexes are particularly effective in Ru-catalyzed asym. hydrogenation of beta-ketoesters to beta-hydroxyesters and Ru-catalyzed asym. hydrogenation of enamides to beta amino acids. Thus, (R)-3,3'-diphenyl-2,2'-bis(diphenylphosphinoxy)-1,1'-binaphthyl was prepd. in five steps starting from (R)-BINOL.

IT 428876-57-7P 428876-61-3P 428876-64-6P 428877-12-7P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of ortho substituted chiral phosphines and phosphinites and their use in asym. catalytic reactions)

RN 428876-57-7 CAPLUS

CN

Phosphine, [(4R)-6,6'-diphenyl[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 428876-61-3 CAPLUS

CN Phosphine, [(5R)-2,2',3,3'-tetrahydro-7,7'-bis(trimethylsilyl)[5,5'-bi-1,4-benzodioxin]-6,6'-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 428876-64-6 CAPLUS

CN

Phosphine, [(5R)-2,2',3,3'-tetrahydro-7,7'-dimethyl[5,5'-bi-1,4-benzodioxin]-6,6'-diyl]bis[bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 428877-12-7 CAPLUS

CN Phosphine, [(4R)-6,6'-dimethyl[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis(3,5-dimethylphenyl)- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

2002:255728 CAPLUS

DOCUMENT NUMBER:

137:154980

TITLE:

Synthesis of new chiral diphosphine ligand

(BisbenzodioxanPhos) and its application in asymmetric

catalytic hydrogenation

AUTHOR (S):

Pai, Cheng-Chao; Li, Yue-Ming; Zhou, Zhong-Yuan; Chan,

Albert S. C.

CORPORATE SOURCE:

Department of Applied Biology and Chemical Technology, Open Laboratory of Chirotechnology of the Institute of Molecular Technology for Drug Design and Synthesis, The Hong Kong Polytechnic University, Hung Hom,

Kowloon, Hong Kong, Peop. Rep. China

SOURCE:

Tetrahedron Letters (2002), 43(15), 2789-2792

CODEN: TELEAY; ISSN: 0040-4039

Elsevier Science Ltd.

PUBLISHER:
DOCUMENT TYPE:
LANGUAGE:

Journal English

OTHER SOURCE(S):

CASREACT 137:154980

GΙ

The new chiral diphosphine ligand [(5,6),(5',6')-bis(1,2-ethylenedioxy)biphenyl-2,2'-diyl]bis(diphenylphosphine) (I;
BisbenzodioxanPhos) was successfully prepd. and used in Ru-catalyzed asym.
hydrogenation of 2-(6'-methoxy-2'-naphthyl)propenoic acid and .beta.-keto
esters with high enantioselectivity (92.2% and up to 99.5% ee, resp.).

IT 445467-61-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and hydrogen peroxide oxidn. of)

RN 445467-61-8 CAPLUS

Ι

CN Phosphine, [(5R)-2,2',3,3'-tetrahydro[5,5'-bi-1,4-benzodioxin]-6,6'-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

2001:830729 CAPLUS 135:371876

DOCUMENT NUMBER: TITLE:

Process for the preparation of 1-menthol via

successive enantioselective hydrogenation reactions

catalyzed by transition metal complexes

INVENTOR(S):

Sayo, Noboru; Matsumoto, Takaji

PATENT ASSIGNEE(S):

Takasago International Corporation, Japan

SOURCE:

Eur. Pat. Appl., 25 pp.

DOCUMENT TYPE:

Patent

CODEN: EPXXDW

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

EP 1153908 A2 20011114 EP 2001-401180 20010509

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

US 2002007094 A1 20020117 US 2001-849306 20010507

US 6342644 B1 20020129

JP 2002030009 A2 20020129 JP 2001-138438 20010509 PRIORITY APPLN. INFO.: JP 2000-137388 A 20000510

OTHER SOURCE(S): CASREACT 135:371876; MARPAT 135:371876

A method was presented for the prodn. of 1-menthol via hydrogenation of piperitenone catalyzed by a transition metal complex of a specified optically active phosphine to produce pulegone, hydrogenation of the obtained pulegone with a ruthenium-phosphine-amine complex in the presence of base to obtain pulegol, and further hydrogenation of the pulegol with a transition metal catalyst . Thus, piperitenone in the presence of  $[Rh(cod)Cl]_2$ , (S)-2,2'-bis[di(3,5-xylyl)phosphino]-1,1'-binaphthyl, andMe(CH2)5P+Ph3Br- in THF was reacted at 50.degree. for 18 h. under a hydrogen pressure of 3 MPa to give (R)-pulegone in 90.1% yield and 97.0% ee. Then, (R)-pulegone in the presence of RuCl2(PPh3)3, H2NCH2CH(OH)CH2NH2, and KOH in 2-propanol was reacted at 25.degree. for 3 h. under a hydrogen pressure of 2 MPa to give (1R)-cis-pulegol in 85% yield. Finally, (1R)-cis-pulegol in the presence of Pd/C in AcOEt was stirred at 60.degree. for 5 h. under a hydrogen pressure of 2 MPa to give a mixt. 1-menthol and (+)-neoisomenthol in a 91:9 diastereomeric ratio and 90% yield.

IT 210169-40-7

RL: CAT (Catalyst use); USES (Uses)

(process for the prepn. of 1-menthol via successive stereoselective hydrogenation reactions catalyzed by transition metal complexes)

RN 210169-40-7 CAPLUS

CN Phosphine, [(4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis[3,5-bis(1,1-dimethylethyl)-4-methoxyphenyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:262994 CAPLUS

DOCUMENT NUMBER: 135:76619

TITLE: New chiral diphosphine ligands designed to have a

narrow dihedral angle in the biaryl backbone

AUTHOR(S): Saito, Takao; Yokozawa, Tohru; Ishizaki, Takero;

Moroi, Takashi; Sayo, Noboru; Miura, Takashi;

Kumobayashi, Hidenori

CORPORATE SOURCE: Central Research Laboratory, Takasago International

Corporation, Kanagawa, 254-0073, Japan

SOURCE: Advanced Synthesis & Catalysis (2001), 343(3), 264-267

CODEN: ASCAF7; ISSN: 1615-4150

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:76619

AB A series of novel optically active diphosphine ligands,

(4,4'-bi-1,3-benzodioxole)-5,5'-diyl-bis(diarylphosphine)s, which are called SEGPHOS, has been designed and synthesized with dihedral angles in the Ru complexes being less than that in the corresponding BINAP-Ru complex. The stereorecognition abilities of SEGPHOS-Ru complex catalysts in the asym. catalytic hydrogenation of a wide variety of carbonyl compds.

are superior to those obsd. with BINAP-Ru complex catalysts.

IT 244261-66-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and ruthenium complexation of)

RN 244261-66-3 CAPLUS

CN Phosphine, [(4R)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS

L5 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:53872

DOCUMENT NUMBER: 134:237356

TITLE: Highly enantioselective palladium-catalyzed ene-type

cyclization of a 1,6-enyne

AUTHOR(S): Hatano, Manabu; Terada, Masahiro; Mikami, Koichi CORPORATE SOURCE: Dep. Appl. Chem., Grad. sch. Sci. Eng., Tokyo Inst.

Technol., Tokyo, 152-8552, Japan

SOURCE: Angewandte Chemie, International Edition (2001),

40(1), 249-253

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal LANGUAGE: English

GI

Ι

The authors developed a highly efficient palladium(II)-catalyzed ene-type carbocyclization of 1,6-enyne MeCH=C(Me)CH2OCH2C.tplbond.CCO2Me leading to enantiopure furan (I). This highly enantioselective catalysis is applicable for the construction of an enantioenriched quaternary chiral center. Possible mechanisms including neutral and cationic intermediate have been proposed.

IT 210169-57-6 244261-66-3

RL: CAT (Catalyst use); USES (Uses) (chiral ligand; enantioselective palladium-catalyzed ene-type cyclization of a 1,6-enyne)

RN 210169-57-6 CAPLUS

CN Phosphine, [(4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis(3,5-dimethylphenyl)- (9CI) (CA INDEX NAME)

RN 244261-66-3 CAPLUS

CN Phosphine, [(4R)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 10 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

1999:722753 CAPLUS

DOCUMENT NUMBER:

131:331431

TITLE:

Preparation of ruthenium iodo complexes containing optically active bidentate phosphine ligands as stereoselective hydrogenation catalysts for

4-methylene-2-oxetanone

INVENTOR(S):

Okeda, Yoshiki; Hashimoto, Tsutomu; Hori, Yoji;

Hagiwara, Toshimitsu

PATENT ASSIGNEE(S):

Takasago International Corporation, Japan

SOURCE:

Eur. Pat. Appl., 57 pp.

DOCUMENT TYPE:

CODEN: EPXXDW Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION N	O. DATE
EP 955303	A2 199911	.0 EP 1999-40112	0 19990507
	A3 200101	03	
R: AT, BE,	CH, DE, DK, E	FR, GB, GR, IT, LI,	LU, NL, SE, MC, PT,
JP 11322734	LT, LV, FI, R		_
· · · · ·		34 JP 1998-14223	
JP 2000288399	A2 200010	.7 JP 1999-93644	19990331
	A 200003	8 US 1999-30775	
EP 1041079	A2 200010	4 EP 2000-40084	7 20000328
EP 1041079	A3 200101	3	
R: AT, BE,	CH, DE, DK, E	, FR, GB, GR, IT, LI,	LU, NL, SE, MC, PT,
IE, SI,	LT, LV, FI, R	1	
PRIORITY APPLN. INFO	.:	JP 1998-142233	A 19980508
		JP 1999-93644	A 19990331
OTHER SOURCE(S):	MARPAT 13		19990331

$$R^2$$
 $PR^1R^1$ 
 $R^3$ 
 $PR^1R^1$ 
 $R^2$ 
 $R^2$ 
 $R^2$ 

Provided are ruthenium iodo complexes contg. optically active bidentate AΒ phosphine ligands, [Ru-(I)q-(T1)n(sol)r(L)]m(T2)p(I)s (T1 = carboxylate anion, sol = polar solvent, L = optically active bidentate phosphine ligand, T2 = anion different from halide and carboxylate anion, n = 0-1, r = 0, 3, 4, m = 1-2, q = 0-1, m = 2, 1, or 1.5, p = 0 or 1, s = 0-2). The optically active bidentate phosphine ligands include diphosphines I (R1 = various (un) substituted aryl groups; R2, R3 = H, halo, C1-4 alkyl, C1-4 alkoxy, or R2R3 = 5- or 6-membered ring). The complexes may be prepd. by

reaction of [RuI(arene)(L)]I or [RuI2(arene)]2 with an alkali or alk. earth metal carboxylate salt in a polar non-nitrile-type solvent. The ruthenium complexes are catalysts for the asym. hydrogenation of 4-methylene-2-oxetanone to give chiral 4-methyl-2-oxetanone. Thus, reaction of [RuI2(p-cymene)]2 with (S)-BINAP (BINAP = 2,2'-bis(diphenylphosphino)1,1'-binaphthyl) in MeOH under N2 at 55.degree. for 16 h, followed by removal of MeOH, and further reaction with NaOAc in CH2Cl2/H2O under N2 for 16 h afforded [RuI(MeCO2){(S)-BINAP}]2 in 97% yield. Hydrogenation of 4-methylene-2-oxetanone in THF with added deaerated H2O in the presence of [RuI(MeCO2){(S)-BINAP}]2 afforded (R)-4-methyl-2-oxetanone in 94% e.e.

IT 210169-54-3 210169-57-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of ruthenium iodo complexes contg. optically active bidentate phosphine ligands)

RN 210169-54-3 CAPLUS

CN Phosphine, (4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[diphenyl- (9CI) (CA INDEX NAME)

RN 210169-57-6 CAPLUS

CN Phosphine, [(4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis(3,5-dimethylphenyl)- (9CI) (CA INDEX NAME)

IT 210169-54-3DP, ruthenium iodo complexes with/without carboxylato ligands

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. as catalysts for stereoselective hydrogenation of

methyleneoxetanone)

RN210169-54-3 CAPLUS

CN Phosphine, (4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[diphenyl- (9CI) (CA INDEX NAME)

ANSWER 9 OF 10 CAPLUS COPYRIGHT 2003 ACS L5

ACCESSION NUMBER:

1999:631421 CAPLUS

DOCUMENT NUMBER:

131:251749

TITLE:

Preparation of ruthenium chiral [4,4'-bi-1,3benzodioxole]-5,5'-diyldiphosphine complexes as

asymmetric hydrogenation catalysts

INVENTOR(S):

Sayo, Noboru; Saito, Takao; Yokozawa, Tohru Takasago International Corporation, Japan

PATENT ASSIGNEE(S): SOURCE:

Eur. Pat. Appl., 11 pp. CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
				~
EP 945457	A2	19990929	EP 1999-400657	19990317
EP 945457	<b>A</b> 3	20001213		
R: AT, BE,	CH, DE	, DK, ES, FR	, GB, GR, IT, LI, LU	, NL, SE, MC, PT,
IE, SI,	LT, LV	, FI, RO		
JP 11269185	A2	19991005	JP 1998-92174	19980323
US 6313317	B1	20011106	US 1999-273260	19990322
PRIORITY APPLN. INFO	.:		JP 1998-92174 A	19980323
OTHER SOURCE(S):	MA	RPAT 131:251	749	

GΙ

AB Disclosed is a novel ruthenium-phosphine complex usable as the catalyst giving a high enantiomer excess in an asym. reaction and a method for producing the complex, the method ensuring the synthesis of the complex as

a pure and single product without the necessity of refining. The ruthenium-phosphine complex is represented by the general formula  $[{RuX(L)}_2(.mu.-X)_3]-[(R2)_2NH2]+(I)$  wherein R2 represents a hydrogen atom, an alkyl group having 1-5 carbon atoms, a cycloalkyl group, a Ph group which may have a substituted group or a benzyl group which may have a substituted group and L represents a diphosphine ligand (II) wherein R1 represents a Ph group or a naphthyl group which may have a substituted group, a cyclohexyl group or a cyclopentyl group and X represents a halogen atom. The method for prepg. a ruthenium-phosphine complex represented by the above general formula I was characterized in that a ruthenium complex [RuX(arene)(L)]X (wherein X, arene, L and R1 are the same as defined above) and an ammonium salt (R2)2NH.cntdot.RX (wherein X and R2 are the same as defined above) were used as starting material and are reacted with each other. Thus, [{RuCl((R)-SEGPHOS)}2(.mu.-Cl)3][Me2NH2] (SEGPHOS = II, R1 = Ph) was prepd. from [RuCl2(benzene)]2 and Me2NH.cntdot.HCl in 95% yield and was shown to catalyze the hydrogenation of 2-oxopropanol to 1,2-dihydroxypropanol in 95% yield with 98% ee.

IT 210169-54-3 244261-66-3 244261-68-5 244261-70-9 244261-72-1 244261-75-4 244261-78-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for prepn. of ruthenium chiral (bibenzodioxole)diyldiphosphin
e complexes as asym. hydrogenation catalysts)

RN 210169-54-3 CAPLUS

CN Phosphine, (4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[diphenyl- (9CI) (CA INDEX NAME)

RN 244261-66-3 CAPLUS CN Phosphine, [(4R)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 244261-68-5 CAPLUS CN Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[bis(4-methylphenyl)-(9CI) (CA INDEX NAME)

RN 244261-70-9 CAPLUS

CN Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[bis(3,5-dimethylphenyl)-(9CI) (CA INDEX NAME)

RN 244261-72-1 CAPLUS

CN Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[bis(4-methoxy-3,5-dimethylphenyl)- (9CI) (CA INDEX NAME)

RN 244261-75-4 CAPLUS

CN Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[diphenyl- (9CI) (CA INDEX NAME)

RN 244261-78-7 CAPLUS

CN Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[bis[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 1998:466349 CAPLUS

DOCUMENT NUMBER:

129:124055

TITLE:

Preparation of chiral (5,6), (5',6')-bis(3,4-

methylenedioxy)biphenyl-2,2'-diylphosphine compound, intermediate for preparing the same, transition metal complex having the same diphosphine compound as ligand

and asymmetric hydrogenation catalyst

INVENTOR(S):

Saito, Takao; Yokozawa, Tohru; Xiaoyaong, Zhang; Sayo,

Noboru

PATENT ASSIGNEE(S):

Takasago International Corp., Japan

SOURCE:

Eur. Pat. Appl., 17 pp. CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
		<b></b>		
EP 850945	A1	19980701	EP 1997-403152	19971224
EP 850945	B1	20021127		13371221
R: AT, BE,	CH, DE,	DK, ES, FR,	GB, GR, IT, LI, LU	, NL, SE, MC, PT.
IE, SI,	LT, LV,	FI, RO		, , , ==,
JP 10182678	A2	19980707	JP 1996-359818	19961226
JP 3148136	B2 :	20010319		
US 5872273	<b>A</b> :	19990216	US 1997-996405	19971222
PRIORITY APPLN. INFO	.:	J	P 1996-359818 A	19961226
OTHER SOURCE(S):	MAR	PAT 129:12405	5	
GI				

I

The present invention provides a novel diphosphine compd. of the formula AB (I; R1 and R2 represent independently cycloalkyl, unsubstituted or substituted Ph, or five-membered heteroarom. ring residue). The compd. is useful as a ligand having the excellent performance (diastereoselectivity, enantioselectivity, and catalytic activity) for an asym. reaction, in particular, asym. hydrogenation catalyst. Thus, diphenyl[2-iodo-(3,4)methylenedioxyphenyl]phosphine (prepn. given) was coupled to each other in the presence of Cu powder in DMF at 140.degree. for 8 h to give (.+-.)-[(5,6)(5',6')-bis(methylenedioxy)biphenyl-2,2'diyl]bis(diphenylphosphine oxide) [(.+-.)-II]. Optical resoln. of the latter compd. by cyclocondensation with (-)-dibenzoyl-L-tartaric acid in EtOAc at 60.degree. for 30 min followed by alkali hydrolysis gave (-)-II, which was reduced by SiCl4 in the presence of dimethylaniline in toluene at 100.degree. for 4 h to give (-)-I (R1 = R2 = Ph) [(-)-SEGPHOS]. [Ru(COD)Cl2]2, (-)-SEGPHOS, Et3N, and toluene was refluxed for 15 h under N followed distg. off the solvent and vacuum drying to give the catalyst Ru2Cl4[(-)-SEGPHOS]2NEt3. The latter catalyst, 2-oxo-1-propanol, and MeOH was autoclaved with stirring at H pressure 10 atm and 65.degree. for 16 to give optically active 1,2-propanediol of 97.4%ee in 99.8%.

IT 210169-38-3P 210169-40-7P 210169-42-9P 210169-44-1P 210169-46-3P 210169-48-5P 210169-50-9P 210169-52-1P

RL: CAT (Catalyst use); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of chiral bis(methylenedioxy)biphenyldiylphosphine and their transition metal complexes as ligands and asym. hydrogenation catalysts)

RN 210169-38-3 CAPLUS

CN Phosphine, [(4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis(4-methoxy-3,5-dimethylphenyl)- (9CI) (CA INDEX NAME)

RN 210169-40-7 CAPLUS

CN Phosphine, [(4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis[3,5-bis(1,1-dimethylethyl)-4-methoxyphenyl]- (9CI) (CA INDEX NAME)

RN210169-42-9 CAPLUS

Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[bis[3,5-bis(1,1-dimethylethyl)phenyl]-, (+)- (9CI) (CA INDEX NAME) CN

RN

210169-44-1 CAPLUS
Phosphine, [(4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis(4-methylphenyl)- (9CI) (CA INDEX NAME) CN

210169-46-3 CAPLUS RNCN

Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[bis[4-(1,1-dimethylethyl)phenyl]-, (+)- (9CI) (CA INDEX NAME)

RN

210169-48-5 CAPLUS
Phosphine, [(4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME) CN

RN 210169-50-9 CAPLUS
CN Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[bis(4-chlorophenyl)-,
(+)- (9CI) (CA INDEX NAME)

RN 210169-52-1 CAPLUS
CN Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[dicyclohexyl-, (+)-(9CI) (CA INDEX NAME)

IT 210169-54-3P 210169-57-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of chiral bis(methylenedioxy)biphenyldiylphosphine and their transition metal complexes as ligands and asym. hydrogenation catalysts)

RN 210169-54-3 CAPLUS

CN Phosphine, (4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[diphenyl- (9CI) (CA INDEX NAME)

RN 210169-57-6 CAPLUS

CN Phosphine, [(4S)-[4,4'-bi-1,3-benzodioxole]-5,5'-diyl]bis[bis(3,5-dimethylphenyl)- (9CI) (CA INDEX NAME)

3

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE RELOADED ON OCTOBER 20, 2002

FILE COVERS 1779 TO 2001.
\*\*\* FILE CONTAINS 8,374,887 SUBSTANCES \*\*\*

- >>> For the revised summary sheet please see:
  http://info.cas.org/ONLINE/DBSS/beilsteinss.html <<<</pre>
- >>> PLEASE NOTE: Reaction and substance documents are stored in
  different file segments. Use separate queries to search for
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  information you have the option to chose the file segment.
  (Use "/XXX.SUB" to search for a bibliographic term in
  substance documents. To restrict the search to reaction
  documents use "/XXX.RX".)
  For additional information see HELP RXS. <<<</pre>

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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=> d his
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(FILE 'HOME' ENTERED AT 15:40:00 ON 31 JAN 2003)

FILE 'REGISTRY' ENTERED AT 15:40:06 ON 31 JAN 2003

L1STRUCTURE UPLOADED

L2STRUCTURE UPLOADED

L31 S L2

L421 S L2 FULL

FILE 'CAPLUS' ENTERED AT 16:05:27 ON 31 JAN 2003

L5 10 S L4

FILE 'BEILSTEIN' ENTERED AT 16:06:59 ON 31 JAN 2003

=> s 14 full

L6 0 L4

=> s l1 full

FULL SEARCH INITIATED 16:07:27 FILE 'BEILSTEIN' FULL SCREEN SEARCH COMPLETED - 297 TO ITERATE

100.0% PROCESSED 297 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.03

L7 0 SEA SSS FUL L1

=> s 12 full

FULL SEARCH INITIATED 16:07:36 FILE 'BEILSTEIN' FULL SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED

8 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.05

L8 3 SEA SSS FUL L2

=> d ide

ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL L8

Beilstein Records (BRN):

Chemical Name (CN):

8893429

DTBM-SEGPHOS

Autonom Name (AUN):

5,5'-bis-<bis-(3,5-di-tert-butyl-4-methoxy-

phenyl)-phosphanyl>-

<4,4'>bi<benzo<1,3>dioxolyl>

Molec. Formula (MF):

C74 H100 O8 P2

Molecular Weight (MW): Lawson Number (LN):

1179.55

Lawson Number (LN):

24014, 16730, 289

Compound Type (CTYPE): Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 7524026 Tautomer ID (TAUTID): 8359415

Tautomer ID (TAUTID):

Entry Date (DED):

2001/10/25

Update Date (DUPD):

2001/10/25

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \* Field Availability:

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Occurrence
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    BRN Beilstein Records
            Chemical Name
    AUN
            Autonomname
    MF
            Molecular Formula
    FW Formular Weight
LN Lawson Number
CTYPE Compound Type
CONSID Constitution ID
                                                     1
    TAUTID Tautomer ID
    ED
            Entry Date
    UPD
            Update Date
   This substance also occurs in Reaction Documents:
    Code
                                            Occurrence
    RX Reaction Documents
    RXPRO Substance is Reaction Product
                                                     1
=> d frxpro
    ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL
Reaction:
    Reaction ID (.ID):
                                8857498
    Reactant BRN (.RBRN):
                               8893664
    Reactant (.RCT):
                                5,5'-bis-<bis-(3,5-di-tert-butyl-4-methoxy-
                                phenyl)-phosphinoyl>-
                                 <4,4'>bi<benzo<1,3>dioxolyl>
    Product BRN (.PBRN):
                                8893429
    Product (.PRO):
                                 5,5'-bis-<bis-(3,5-di-tert-butyl-4-methoxy-
                                 phenyl) -phosphanyl>-
                                 <4,4'>bi<benzo<1,3>dioxolyl>
    No. of React. Details (.NVAR): 1
Reaction Details:
    Reaction RID (.RID):
                                8857498.1
    Reaction Classification (.CL): Multistage
    Nr. of Stages (.SNR):
    Stage 1
    Reagent (.RGT):
                              Cl3SiH, N,N-dimethylaniline
    Solvent (.SOL):
                                toluene
    Other Conditions (.COND):
                               Heating
    Stage 2
    Reagent (.RGT):
                                aq. NaOH
    Solvent (.SOL):
                                toluene
    Temperature (.T):
                                 20 Cel
    Reference(s):
    1. Saito, Takao; Yokozawa, Tohru; Ishizaki, Takero; Moroi, Takashi; Sayo,
      Noboru; Miura, Takashi; Kumobayashi, Hidenori, Adv.Synth.Catal., CODEN:
       ASCAF7, 343(3), <2001>, 264 - 268; BABS-6289823
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1.8

RX

Beilstein Records (BRN): 8889401 Chemical Name (CN): DM-SEGPHOS Autonom Name (AUN): 5,5'-bis-<br/>-dimethyl-phenyl)phosphanyl>-<4,4'>bi<berzo<1,3>dioxolyl> Molec. Formula (MF): C46 H44 O4 P2 Molecular Weight (MW): 722.80 Lawson Number (LN): 24014, 16735 Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 7520808 Tautomer ID (TAUTID): 8350238 Entry Date (DED): 2001/10/25 Update Date (DUPD): 2001/10/25

### Field Availability:

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BRN Beilstein Records	1
CN Chemical Name	1
AUN Autonomname	1
MF Molecular Formula	1
FW Formular Weight	1
LN Lawson Number	2
CTYPE Compound Type	1
CONSID Constitution ID	1
TAUTID Tautomer ID	1
ED Entry Date	1
UPD Update Date	1

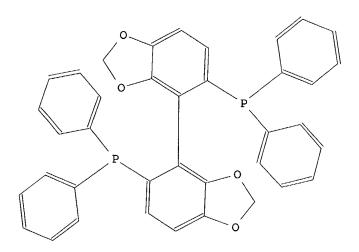
### This substance also occurs in Reaction Documents:

Code	Name	Occurrence
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RX Reaction Documents 1
RXPRO Substance is Reaction Product 1

#### L8 ANSWER 3 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 8886882 Chemical Name (CN): (R)-(+)-(4,4'-bi-1,3-benzodioxole)-5,5'diyl-bis(diphenylphosphine), (R)-SEGPHOS 5,5'-bis-diphenylphosphanyl-Autonom Name (AUN): <4,4'>bi<benzo<1,3>dioxolyl> C38 H28 O4 P2 Molec. Formula (MF): Molecular Weight (MW): 610.58 Lawson Number (LN): 24014, 16731 File Segment (FS): Stereo compound Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 7516387 Tautomer ID (TAUTID): 8344967 Entry Date (DED): 2001/10/25 Update Date (DUPD): 2001/10/25



Fragment Notes:

Stereo Descriptor: R(a)

### Field Availability:

Code	Name	Occurrence
=======		=======================================
BRN	Beilstein Records	1
CN	Chemical Name	2
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
MP	Melting Point	1
NMR	Nuclear Magnetic Resonance	3

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ORP
               Optical Rotatory Power
                                                        1
   This substance also occurs in Reaction Documents:
             Name
                                               Occurrence
     RX Reaction Documents
                                                        1
             Substance is Reaction Product
                                                        1
=> d frxpro
     ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL
L8
Reaction:
RX
     Reaction ID (.ID):
                                    8857498
     Reactant BRN (.RBRN):
                                    8893664
                                    5,5'-bis-<br/>di-tert-butyl-4-methoxy-
     Reactant (.RCT):
                                    phenyl)-phosphinoyl>-
                                   <4,4'>bi<benzo<1,3>dioxolyl>
     Product BRN (.PBRN):
                                    8893429
                                    5,5'-bis-<br/>-di-tert-butyl-4-methoxy-
     Product (.PRO):
                                    phenyl)-phosphanyl>-
                                    <4,4'>bi<benzo<1,3>dioxolyl>
     No. of React. Details (.NVAR):
Reaction Details:
     Reaction RID (.RID):
                                   8857498.1
     Reaction Classification (.CL): Multistage
     Nr. of Stages (.SNR):
     Stage 1
     Reagent (.RGT):
                                   Cl3SiH, N, N-dimethylaniline
     Solvent (.SOL):
                                   toluene
     Other Conditions (.COND):
                                  Heating
     Stage 2
     Reagent (.RGT):
                                   aq. NaOH
     Solvent (.SOL):
                                   toluene
    Temperature (.T):
                                   20 Cel
     Reference(s):
     1. Saito, Takao; Yokozawa, Tohru; Ishizaki, Takero; Moroi, Takashi; Sayo,
       Noboru; Miura, Takashi; Kumobayashi, Hidenori, Adv.Synth.Catal., CODEN:
       ASCAF7, 343(3), <2001>, 264 - 268; BABS-6289823
=> d frxpro 2-3
    ANSWER 2 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL
L8
Reaction:
RX
    Reaction ID (.ID):
                                   8856511
    Reactant BRN (.RBRN):
                                   8890075
    Reactant (.RCT):
                                   5,5'-bis-<br/>-dimethyl-phenyl)-
                                   phosphinoyl>-<4,4'>bi<benzo<1,3>dioxolyl>
    Product BRN (.PBRN):
                                   8889401
    Product (.PRO):
                                   5,5'-bis-<bis-(3,5-dimethyl-phenyl)-
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No. of React. Details (.NVAR):

Reaction Details:

phosphanyl>-<4,4'>bi<benzo<1,3>dioxolyl>

```
RX
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Reaction RID (.RID):
                                      8856511.1
      Reaction Classification (.CL): Multistage
     Nr. of Stages (.SNR):
      Stage 1
     Reagent (.RGT):
                                    Cl3SiH, N,N-dimethylaniline
      Solvent (.SOL):
                                      toluene
     Other Conditions (.COND):
                                     Heating
     Stage 2
     Reagent (.RGT):
                                     aq. NaOH
     Solvent (.SOL):
                                     toluene
     Temperature (.T):
                                      20 Cel
     Reference(s):
     1. Saito, Takao; Yokozawa, Tohru; Ishizaki, Takero; Moroi, Takashi; Sayo,
        Noboru; Miura, Takashi; Kumobayashi, Hidenori, Adv.Synth.Catal., CODEN:
        ASCAF7, 343(3), <2001>, 264 - 268; BABS-6289823
1.8
     ANSWER 3 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL
Reaction:
RX
     Reaction ID (.ID):
                                      8855748
     Reactant BRN (.RBRN):
                                     8887491
     Reactant (.RCT):
                                      (R) - (+) - (4,4'-bi-1,3-benzodioxole) -5,5'-
                                     diyl-bis(diphenylphosphine oxide)
     Product BRN (.PBRN):
                                     8886882
     Product (.PRO):
                                      (R) - (+) - (4, 4'-bi-1, 3-benzodioxole) - 5, 5'-
                                     diyl-bis(diphenylphosphine)
     No. of React. Details (.NVAR): 1
Reaction Details:
RX
     Reaction RID (.RID):
                                     8855748.1
     Reaction Classification (.CL): Multistage
     Yield (.YDT):
                                     95 percent (BRN=8886882)
     Nr. of Stages (.SNR):
     Stage 1
     Reagent (.RGT):
                                     Cl3SiH, N, N-dimethylaniline
     Solvent (.SOL):
                                     toluene
     Time (.TIM):
                                     4 hour(s)
     Temperature (.T):
                                    110 Cel
     Stage 2
     Reagent (.RGT):
                                   aq. NaOH
     Solvent (.SOL):
                                     toluene
     Time (.TIM):
                                     30 min
     Temperature (.T):
                                     20 Cel
     Reference(s):
     1. Saito, Takao; Yokozawa, Tohru; Ishizaki, Takero; Moroi, Takashi; Sayo,
        Noboru; Miura, Takashi; Kumobayashi, Hidenori, Adv.Synth.Catal., CODEN:
        ASCAF7, 343(3), <2001>, 264 - 268; BABS-6289823
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COST IN U.S. DOLLARS
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FULL ESTIMATED COST
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
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CA SUBSCRIBER PRICE
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STRUCTURE FILE UPDATES: 30 JAN 2003 HIGHEST RN 483965-49-7 DICTIONARY FILE UPDATES: 30 JAN 2003 HIGHEST RN 483965-49-7

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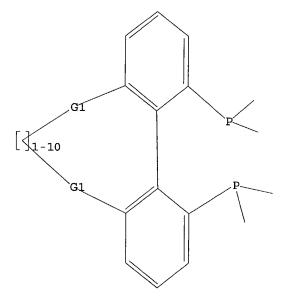
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> Uploading 09991261.str

L9 STRUCTURE UPLOADED

=> d L9 HAS NO ANSWERS L9 STR



G1 O, N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 63 TO ITERATE

100.0% PROCESSED 63 ITERATIONS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

784 TO 1736

PROJECTED ANSWERS:

4 TO 200

L10

4 SEA SSS SAM L9

=> d scan

L10 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(12aR)-6,7-dihydrodibenzo[e,g][1,4]dioxocin-1,12-

diyl]bis[diphenyl- (9CI)

MF C38 H30 O2 P2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> s 19 full

FULL SEARCH INITIATED 16:11:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 992 TO ITERATE

100.0% PROCESSED 992 ITERATIONS

SEARCH TIME: 00.00.01

56 ANSWERS

L11

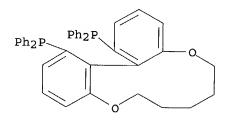
56 SEA SSS FUL L9

=> d scan

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(15aR)-7,8,9,10-tetrahydro-6H-dibenzo[b,d][1,6]dioxacycloundec
in-1,15-diyl]bis[diphenyl- (9CI)

MF C41 H36 O2 P2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(17aR)-7,8,9,10,11,12-hexahydro-6H-

dibenzo[b,d][1,6]dioxacyclotridecin-1,17-diyl]bis[diphenyl- (9CI)

MF C43 H40 O2 P2

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Dibenzo[b,d][1,6]diazacyclotetradecine-6,13-dione, 1,18-

bis(diphenylphosphino)-5,7,8,9,10,11,12,14-octahydro-, (18aR)- (9CI)

MF C44 H40 N2 O2 P2

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Dibenzo[b,d][1,6]diazacyclotetradecine, 1,18-bis(diphenylphosphino)-

5,6,7,8,9,10,11,12,13,14-decahydro-, (18aR)- (9CI)

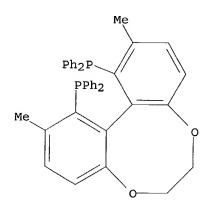
MF C44 H44 N2 P2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(12aR)-6,7-dihydro-2,11-dimethyldibenzo[e,g][1,4]dioxocin-1,12-diyl]bis[diphenyl- (9CI)

MF C40 H34 O2 P2



# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Dibenzo[b,d][1,6]diazecine, 1,14-bis(diphenylphosphino)-5,6,7,8,9,10hexahydro-2,5,10,13-tetramethyl-, (14aR)- (9CI)

MF C44 H44 N2 P2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(13aR)-7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl]bis[diphenyl- (9CI)

MF C39 H32 O2 P2

MF

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 6H-Dibenzo[b,d][1,6]dioxacyclotridecin-6,12(7H)-dione,

1,17-bis(diphenylphosphino)-8,9,10,11-tetrahydro-, (17aR)- (9CI) C43 H36 O4 P2

IN Dibenzo[b,d][1,6]diazacyclododecine-6,11-dione, 1,16bis(diphenylphosphino)-5,7,8,9,10,12-hexahydro-, (16aR)- (9CI)
MF C42 H36 N2 O2 P2

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Phosphine, [(15aR)-6,7,8,9,10,11-hexahydro-5H-dibenzo[b,d][1,6]diazacycloundecine-1,15-diyl]bis[diphenyl-(9CI)
MF C41 H38 N2 P2

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Phosphine, [(13aR)-7,8-dihydro-2,12-diphenyl-6H-dibenzo[f,h][1,5]dioxonin1,13-diyl]bis[diphenyl- (9CI)
MF C51 H40 O2 P2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(14aR)-6,7,8,9-tetrahydro-2,13-dimethyldibenzo[b,d][1,6]dioxec in-1,14-diyl]bis[bis[3,5-bis(1,1-dimethylethyl)phenyl]- (9CI)

MF C74 H102 O2 P2

PAGE 1-A

PAGE 2-A

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, (11aR)-dibenzo[d,f][1,3]dioxepin-1,11-diylbis[diphenyl- (9CI)

MF C37 H28 O2 P2

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 6H-Dibenzo[b,d][1,6]dioxacycloundecin-6,10(7H)-dione, 1,15-bis(diphenylphosphino)-8,9-dihydro-, (15aR)- (9CI)
MF C41 H32 O4 P2

Ph<sub>2</sub>P Ph<sub>2</sub>P O O

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Dibenzo[b,d][1,6]diazecine-6,9-dione, 1,14-bis(diphenylphosphino)-5,7,8,10-tetrahydro-, (14aR)- (9CI)
MF C40 H32 N2 O2 P2

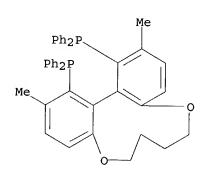
# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 5H-Dibenzo[f,h][1,5]diazonine, 1,13-bis(diphenylphosphino)-6,7,8,9-tetrahydro-, (13aR)- (9CI)
MF C39 H34 N2 P2

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(14aR)-6,7,8,9-tetrahydro-2,13-dimethyldibenzo[b,d][1,6]dioxec
in-1,14-diyl]bis[diphenyl- (9CI)

MF C42 H38 O2 P2



# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(13aR)-7,8-dihydro-2,12-dimethyl-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl]bis[bis(3,5-dimethylphenyl)- (9CI)

MF C49 H52 O2 P2

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Carbamic acid, [3-(triethoxysilyl)propyl]-, (13aR)-1,13bis(diphenylphosphino)-7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin-7-yl ester
(9CI)

MF C49 H53 N O7 P2 Si

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 6H-Dibenzo[f,h][1,5]dioxonin-6,8(7H)-dione, 1,13-bis(diphenylphosphino)-, (13aR)- (9CI)

MF C39 H28 O4 P2

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(20aR)-6,7,8,9,10,11,12,13,14,15-decahydrodibenzo[b,d][1,6]dio
xacyclohexadecin-1,20-diyl]bis[diphenyl- (9CI)

MF C46 H46 O2 P2

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 5H-Dibenzo[d,f][1,3]diazepine, 1,11-bis(diphenylphosphino)-6,7-dihydro-,
(11aR)- (9CI)

MF C37 H30 N2 P2

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, (7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl)bis[bis(4-methylphenyl)-, (-)- (9CI)

MF C43 H40 O2 P2

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(14aR)-6,7,8,9-tetrahydro-2,13-dimethoxydibenzo[b,d][1,6]dioxecin-1,14-diyl]bis[diphenyl- (9CI)

MF C42 H38 O4 P2

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 6H-Dibenzo[f,h][1,5]dioxonin-7-ol, 1,13-bis(diphenylphosphino)-7,8-dihydro, (13aR)- (9CI)

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, [(16aR)-6,7,8,9,10,11-hexahydrodibenzo[b,d][1,6]dioxacyclododec in-1,16-diyl]bis[diphenyl- (9CI)

MF C42 H38 O2 P2

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 56 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Dibenzo[b,d][1,6]dioxacyclotetradecin, 1,18-bis(diphenylphosphino)6,7,8,9,10,11,12,13-octahydro-, (18aR)- (9CI)

MF C44 H42 O2 P2

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=> s 113
L14 6 L13
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=> d ibib abs hitstr 1-6

L14 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 2002:539679 CAPLUS

DOCUMENT NUMBER:

137:109204

TITLE:

Novel process for the synthesis of

5-(4-fluorophenyl)-1-[2-((2R,4R)-4-hydroxy-6-oxotetrahydropyran-2-yl)-ethyl]-2-isopropyl-4-phenyl-1H-

pyrrole-3-carboxylic acid N-phenylamide

INVENTOR (S):

Butler, Donald Eugene; Dejong, Randall Lee; Nelson, Jade Douglas; Pamment, Michael Gerard; Stuk, Timothy

Lee

PATENT ASSIGNEE(S):

Warner-Lambert Company, USA

SOURCE:

PCT Int. Appl., 82 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE: Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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PATENT NO.
                   KIND DATE
                                       APPLICATION NO. DATE
     _____ ____
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    WO 2002055519
                    A2
                          20020718
                                        WO 2001-IB2729
                                                         20011227
    WO 2002055519
                    A3 20020919
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            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,
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    US 2002133026
                    A1 20020919
                                        US 2001-15558
                                                        20011217
    US 6476235
                          20021105
                     B2
PRIORITY APPLN. INFO.:
                                     US 2001-260505P P 20010109
GΙ
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# \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AΒ An improved process for the prepn. of 5-(4-fluorophenyl)-1-[2-((2R,4R)-4-fluorophenyl)]hydroxy-6-oxo-tetrahydropyran-2-yl)ethyl]-2-isopropyl-4-phenyl-1H-pyrrole-3-carboxylic acid phenylamide (I) was disclosed. Morpholine was condensed with Me cyanoacetate (MTBE, 55.degree., 12-18 h), the product reduced to the amine (MeOH, HCl, H2-Pt/C @ 50 psi, 24 h), converted from the hydrochloride to the phenylacetate salt, which was condensed with 2-[2-(4-fluorophenyl)-2-oxo-1-phenylethyl]-4-methyl-3-oxopentanoic acid phenylamide with removal of water (THF, 4-8 mesh 3.ANG. ms, reflux, 24 h) to afford solid II. Et acetoacetate in THF was reacted with NaH at -20.degree. (held at -10.degree. 45 min) followed by n-BuLi at -18.degree. (held at -4.degree. for 90 min) followed by addn. of II at -25.degree. and held at -23.degree. for 20 h yielding, after aq. work-up, A-(CH2)2COCH2COCH2CO2Et (III). Redn. of III with a RuCl2(DMF)n[(+)-Cl-MeO-BIPHEP] complex (MeOH, 1M HBr, H2 @ 50 psi, 65.degree.) to afford .beta.,.delta.-dihydroxy ester IV in a 1:1.5 syn:anti with a .gtoreq.98% enantiomeric excess at the .delta.-hydroxy position in favor of the (R)-configuration (4 diastereomers sepd. by HPLC; Chiralcel-OD-H).

Cyclization/elimination of IV (MeoHaq, KOH, 85.degree.; PhMe, HCl; Ac20, NEt3, DMAP) provides the 6-oxo-3,6-2H-pyran V (98% ee). Treatment of V with BnOH, NaOH at -10.degree. for 19 h followed by hydrogenation (PhMe, 20% Pd(OH)2/C, 50 psi, 50.degree., 16 h) provided VI as a white solid (anti:syn 99:1, enantiomeric excess at the pyran C5 of 99% favoring the (R)-configuration). Alternate methods for several steps were provided. Utilization of VI for the prepn. of atorvastatin calcium was also exemplified. Redn. of .beta.,.delta.-diketo esters reported herein is more stereoselective, can be executed at lower pressures and is more amendable to large-scale manufg. than prior art examples.

IT 301847-88-1D, BIPHEP, BINAP and TunaPhos ruthenium complexes 301847-90-5D, BIPHEP, BINAP and TunaPhos ruthenium complexes RL: CAT (Catalyst use); USES (Uses)

(stereoselective redn. of a .beta.,.delta.-diketo ester leading to 5-(4-fluorophenyl)-1-[2-((2R,4R)-4-hydroxy-6-oxo-tetrahydropyran-2-yl)-ethyl]-2-iso-Pr-4-Ph-1H-pyrrole-3-carboxylic acid N-phenylamide)

RN 301847-88-1 CAPLUS

CN

Phosphine, [(12aR)-6,7-dihydrodibenzo[e,g][1,4]dioxocin-1,12-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-90-5 CAPLUS

CN Phosphine, [(14aR)-6,7,8,9-tetrahydrodibenzo[b,d][1,6]dioxecin-1,14-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN

CN

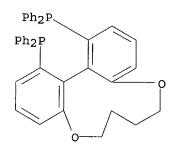
#### IT 301847-88-1 301847-90-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective redn. of a .beta.,.delta.-diketo ester leading to
5-(4-fluorophenyl)-1-[2-((2R,4R)-4-hydroxy-6-oxo-tetrahydropyran-2-yl)ethyl]-2-iso-Pr-4-Ph-1H-pyrrole-3-carboxylic acid N-phenylamide)
301847-88-1 CAPLUS

Phosphine, [(12aR)-6,7-dihydrodibenzo[e,g][1,4]dioxocin-1,12-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-90-5 CAPLUS

> Phosphine, [(14aR)-6,7,8,9-tetrahydrodibenzo[b,d][1,6]dioxecin-1,14diyl]bis[diphenyl- (9CI) (CA INDEX NAME)



L14 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

2002:391724 CAPLUS

DOCUMENT NUMBER:

CN

136:401880

TITLE:

Ortho substituted chiral phosphines and phosphinites

and their use in asymmetric catalytic reactions

INVENTOR (S):

Zhang, Xumu

PATENT ASSIGNEE(S):

The Penn State Research Foundation, USA

SOURCE:

PCT Int. Appl., 122 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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PATENT NO.
                           KIND DATE
                                                     APPLICATION NO. DATE
                                                     -----
      WO 2002040491
                            A1
                                   20020523
                                                     WO 2001-US43779 20011116
           W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
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                RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,
                VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
           RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
      AU 2002016719
                            A5
                                   20020527
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                                                                          20011116
      US 2002128501
                            A1
                                   20020912
                                                     US 2001-991261
                                                                           20011116
PRIORITY APPLN. INFO.:
                                                  US 2000-249537P P
                                                                           20001117
                                                  US 2001-301221P P
                                                                           20010627
                                                 WO 2001-US43779 W
                                                                          20011116
OTHER SOURCE(S):
                              CASREACT 136:401880; MARPAT 136:401880
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GΙ

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3,3'-Substituted chiral biaryl phosphine and phosphinite ligands, I (X, X')= independently (un) substituted alkyl, (un) substituted aryl, alkoxy, organothio, diorganoamido, alkoxycarbonyl, halo, organosilyl, diorganophosphonyl, dialkoxyphosphino; Z, Z1 = independently (un) substituted alkyl, (un) substituted aryl, alkoxy, organothio, diorganoamido, alkoxycarbonyl, halo, organosilyl, diorganophosphonyl, dialkoxyphosphino, bridging group, etc.; Z', Z'', Z1', Z1'' = independently H, (un) substituted alkyl, (un) substituted aryl, alkoxy, organothio, diorganoamido, alkoxycarbonyl, halo, organosilyl, diorganophosphonyl, dialkoxyphosphino, bridging group, etc.; Y, Y' = O, CH2, NH, S, a bond between carbon and phosphorus, etc.; T, T' = (un) substituted alkyl, (un) substituted aryl, alkoxy, etc.) and metal complexes based on such chiral ligands useful in asym. catalysis are disclosed. The metal complexes are useful as catalysts in asym. reactions, such as, hydrogenation, hydride transfer, allylic alkylation, hydrosilylation, hydroboration, hydrovinylation, hydroformylation, hydroformylation, olefin metathesis, hydrocarboxylation, isomerization, cyclopropanation, Diels-Alder reaction, Heck reaction, isomerization, Aldol reaction, Michael addn., epoxidn., Kinetic resoln. and [m + n]cycloaddn. The metal complexes are particularly effective in Ru-catalyzed asym. hydrogenation of beta-ketoesters to beta-hydroxyesters and Ru-catalyzed asym. hydrogenation of enamides to beta amino acids. Thus, (R) -3,3'-diphenyl-2,2'-bis(diphenylphosphinoxy)-1,1'-binaphthyl was prepd. in five steps starting from (R)-BINOL.

11 170 Sceps Starting from (R)-BINOL. 428877-93-4P 428877-94-5P 428877-95-6P 428877-96-7P 428877-97-8P 428878-00-6P 428878-01-7P 428878-02-8P 428878-03-9P 428878-04-0P 428878-05-1P 428878-06-2P 428878-07-3P 428878-08-4P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of ortho substituted chiral phosphines and phosphinites and their use in asym. catalytic reactions)

RN 428877-93-4 CAPLUS

CN

Phosphine, [(14aR)-6,7,8,9-tetrahydro-2,13-dimethyldibenzo[b,d][1,6]dioxec in-1,14-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 428877-94-5 CAPLUS

CN

6H-Dibenzo[f,h][1,5]dioxonin-2,12-dicarboxylic acid, 1,13-bis(diphenylphosphino)-7,8-dihydro-, diethyl ester, (13aR)- (9CI) (CA INDEX NAME)

RN 428877-95-6 CAPLUS

CN Phosphine, [(13aR)-7,8-dihydro-2,12-diphenyl-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 428877-96-7 CAPLUS

CN Phosphine, [(14aR)-6,7,8,9-tetrahydro-2,13-diphenyldibenzo[b,d][1,6]dioxec in-1,14-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 428877-97-8 CAPLUS

CN Phosphine, [(12aR)-6,7-dihydro-2,11-dimethyldibenzo[e,g][1,4]dioxocin-1,12-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 428878-00-6 CAPLUS

CN Dibenzo[b,d][1,6]diazecine, 1,14-bis(diphenylphosphino)-5,6,7,8,9,10-hexahydro-2,13-dimethyl-, (14aR)- (9CI) (CA INDEX NAME)

RN 428878-01-7 CAPLUS

CN Phosphine, [(14aR)-6,7,8,9-tetrahydro-2,13-dimethoxydibenzo[b,d][1,6]dioxecin-1,14-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 428878-02-8 CAPLUS

CN Phosphine, [(14aR)-6,7,8,9-tetrahydro-2,13-dimethyldibenzo[b,d][1,6]dioxec in-1,14-diyl]bis[bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 428878-03-9 CAPLUS

CN Phosphine, [(13aR)-7,8-dihydro-2,12-dimethyl-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl]bis[bis(3,5-dimethylphenyl)- (9CI) (CA INDEX NAME)

RN 428878-04-0 CAPLUS

CN Phosphine, [(15aR)-7,8,9,10-tetrahydro-2,14-dimethyl-6H-dibenzo[b,d][1,6]dioxacycloundecin-1,15-diyl]bis[dicylohexyl- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 428878-05-1 CAPLUS

CN Phosphine, [(14aR)-6,7,8,9-tetrahydro-2,13-dimethyldibenzo[b,d][1,6]dioxec in-1,14-diyl]bis[bis[3,5-bis(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

PAGE 2-A

RN

428878-06-2 CAPLUS
Phosphine, [(14aR)-6,7,8,9-tetrahydro-2,13-dimethyldibenzo[b,d][1,6]dioxecin-1,14-diyl]bis[bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME) CN

RN 428878-07-3 CAPLUS

CN Dibenzo[b,d][1,6]diazecine, 1,14-bis(diphenylphosphino)-5,6,7,8,9,10-hexahydro-2,5,10,13-tetramethyl-, (14aR)- (9CI) (CA INDEX NAME)

RN 428878-08-4 CAPLUS

CN Phosphine, [(11aR)-2,10-dimethoxydibenzo[d,f][1,3]dioxepin-1,11-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

2001:597876 CAPLUS

DOCUMENT NUMBER:

135:180880

TITLE:

Chiral ferrocene phosphines and their use in

asymmetric catalytic reactions

INVENTOR(S):

Zhang, Xumu

PATENT ASSIGNEE(S):

The Penn State Research Foundation, USA

SOURCE:

PCT Int. Appl., 107 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Fralial

FAMILY ACC. NUM. COUNT:

English

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2001058588 A1 20010816 WO 2001-US4442 20010209

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,

SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,

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BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002091280 A1 20020711 US 2001-781083 20010209 EP 1257360 A1 20021120 EP 2001-909127 20010209

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.: US 2000-181448P P 20000210

US 2000-214167P P 20000626

WO 2001-US4442 W 20010209

OTHER SOURCE(S): CASREACT 135:180880; MARPAT 135:180880

Metal complexes with ferrocene anchored chiral ligands are useful in asym. catalysis, such as hydrogenation and allylic alkylation. Thus, (S,S,S,S) ferrocene amide phosphine was prepd. from (1S,2S)diaminocyclohexane and chiral carboxyferrocenyl di-Ph phosphine and used in combination with (.eta.3-allyl)PdCl2 to catalysis allylic alkylation between 2-cyclohexenyl acetate and di-Me malonate to give [(1R)-2-cyclohexen-1-yl]propanedioic acid di-Me ester in 61% and 20% ee

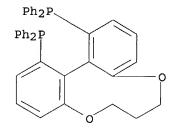
(R). IT 301847-89-2

RL: CAT (Catalyst use); USES (Uses)

(chiral ferrocene phosphines for asym. alkylation reaction catalysis)

RN 301847-89-2 CAPLUS

Phosphine, [(13aR)-7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin-1,13-CN diyl]bis[diphenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:

2001:319498 CAPLUS

DOCUMENT NUMBER:

134:326631

TITLE:

Optically active diphosphine compound, production intermediates therefor, transition metal complex containing the compound as ligand and asymmetric hydrogenation catalyst containing the complex

INVENTOR (S):

Yokozawa, Tohru; Sayo, Noboru; Saito, Takao; Ishizaki,

Takero

PATENT ASSIGNEE(S):

Takasago International Corporation, Japan

SOURCE: Eur. Pat. Appl., 19 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE \_\_\_\_ -----EP 1095946 20010502 A1 EP 2000-402997 20001027 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

JP 2001131192 A2 20010515 JP 1999-309976 19991029 US 6333291 B1 20011225 US 2000-698208 20001030 PRIORITY APPLN. INFO:: JP 1999-309976 A 19991029

OTHER SOURCE(S): MARPAT 134:326631

GΙ

Ι

This invention provides a novel diphosphine compd. which is useful as a ligand of catalysts for asym. synthesis reactions, particularly asym. hydrogenation reaction. Particularly, it provides a diphosphine compd. I (R1, R2 = each independently represents a cycloalkyl group, an unsubstituted or substituted Ph group or a five-membered arom. heterocycle residue). Thus, reaction of I (L, R1 = R2 = Ph), prepd. in 5 steps starting from 3-bromophenol, with [Ru(p-cymene)I2]2 gave [RuI(p-cymene)(L)] which was used as catalyst for asym. hydrogenation of Me benzoylacetate.

IT 337359-59-8P 337359-61-2P 337359-92-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(ruthenium complex with optically active diphosphine ligand catalyzed asym. hydrogenation of)

RN 337359-59-8 CAPLUS

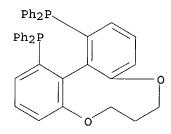
CN Phosphine, (7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl)bis[bis(3,5-dimethylphenyl)-, (-)- (9CI) (CA INDEX NAME)

RN 337359-61-2 CAPLUS

CN Phosphine, (7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl)bis[bis(4-

RN 337359-92-9 CAPLUS

CN Phosphine, (7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl)bis[diphenyl-, (-)- (9CI) (CA INDEX NAME)



RECORD. ALL CITATIONS AV

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: DOCUMENT NUMBER:

REFERENCE COUNT:

2001:228894 CAPLUS

TITLE:

134:266437

Chiral phosphines, transition metal complexes thereof

and uses thereof in asymmetric reactions

INVENTOR(S):

Zhang, Xumu

PATENT ASSIGNEE(S):

Penn State Research Foundation, USA

SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DAT	ГЕ	APPLICAT	ION NO.	DATE	
HU, ID, LU, LV,		T, AU, AZ, 1 K, DM, DZ, 1 S, JP, KE, 1 G, MK, MN, 1	BA, BB, BG EE, ES, FI KG, KP, KR MW, MX, MZ	BR, BY, GB, GD, KZ, LC, NO, NZ,	BZ, CA, GE, GH, LK, LR, PL, PT,	CH, CN, GM, HR, LS, LT, RO, RU,

YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG Α1 20020619 EP 2000-965136 20000919 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL PRIORITY APPLN. INFO.: US 1999-154845P P 19990920 WO 2000-US25635 W 20000919 OTHER SOURCE(S): CASREACT 134:266437; MARPAT 134:266437 GΙ

AB Chiral ligands and transition metal complexes based on such chiral ligands useful in asym. catalysis are disclosed. The chiral ligands include chiral C1-C6-TunaPhos ligands I (n = 1-6). The ruthenium TunaPhos complex reduces ketones to the corresponding alcs. with 95-99.6 \$enantioselectivity. The transition metal complexes of the chiral ligands are useful in asym. reactions such as asym. hydrogenation, hydride transfer, hydrosilylation, hydroboration, hydrovinylation, hydroformylation, hydrocarboxylation, isomerization, allylic alkylation, cyclopropanation, Diels-Alder reaction, Heck reaction, isomerization, Aldol reaction, Michael addn. and epoxidn. reactions.

301847-87-0P, (R)-C1-TunaPhos 301847-88-1P, (R) -C2-TunaPhos 301847-89-2P, (R) -C3-TunaPhos 301847-90-5P, (R)-C4-TunaPhos 301847-91-6P, (R) -C5-TunaPhos 301847-92-7P, (R) -C6-TunaPhos RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. as cocatalyst in transition metal complex catalyzed asym. reactions)

RN 301847-87-0 CAPLUS

Phosphine, (11aR)-dibenzo[d,f][1,3]dioxepin-1,11-diylbis[diphenyl- (9CI) CN (CA INDEX NAME)

IT

RN 301847-88-1 CAPLUS

CN Phosphine, [(12aR)-6,7-dihydrodibenzo[e,g][1,4]dioxocin-1,12-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-89-2 CAPLUS

CN Phosphine, [(13aR)-7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-90-5 CAPLUS

CN Phosphine, [(14aR)-6,7,8,9-tetrahydrodibenzo[b,d][1,6]dioxecin-1,14-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-91-6 CAPLUS

CN Phosphine, [(15aR)-7,8,9,10-tetrahydro-6H-dibenzo[b,d][1,6]dioxacycloundecin-1,15-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-92-7 CAPLUS

CN Phosphine, [(16aR)-6,7,8,9,10,11-hexahydrodibenzo[b,d][1,6]dioxacyclododec in-1,16-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

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IT
     331768-59-3 331768-62-8 331768-63-9
     331768-64-0 331768-65-1 331768-66-2
     331768-67-3 331768-68-4 331768-69-5
     331768-70-8 331768-71-9 331769-04-1
     331769-05-2 331769-06-3 331769-07-4
     331769-08-5 331769-09-6 331769-13-2
     331769-15-4 331769-16-5 331769-17-6
     331769-18-7 331769-19-8 331769-20-1
     331769-21-2 331769-22-3 331776-92-2
     RL: CAT (Catalyst use); USES (Uses)
        (prepn. of chiral diphosphines as cocatalyst in transition metal
        complex catalyzed asym. reactions)
     331768-59-3 CAPLUS
RN
CN
     Dibenzo[d,f][1,3]dioxepin-6-one, 1,11-bis(diphenylphosphino)-, (11aR)-
           (CA INDEX NAME)
```

RN 331768-62-8 CAPLUS

CN 6H-Dibenzo[f,h][1,5]dioxonin-6,8(7H)-dione, 1,13-bis(diphenylphosphino)-, (13aR)- (9CI) (CA INDEX NAME)

RN 331768-63-9 CAPLUS

CN Dibenzo[b,d][1,6]dioxecin-6,9-dione, 1,14-bis(diphenylphosphino)-7,8-dihydro-, (14aR)- (9CI) (CA INDEX NAME)

RN 331768-64-0 CAPLUS

CN 6H-Dibenzo[b,d][1,6]dioxacycloundecin-6,10(7H)-dione, 1,15-bis(diphenylphosphino)-8,9-dihydro-, (15aR)- (9CI) (CA INDEX NAME)

RN 331768-65-1 CAPLUS

CN Dibenzo[b,d][1,6]dioxacyclododecin-6,11-dione, 1,16-bis(diphenylphosphino)-7,8,9,10-tetrahydro-, (16aR)- (9CI) (CA INDEX NAME)

RN 331768-66-2 CAPLUS
CN 6H-Dibenzo[b,d][1,6]dioxacyclotridecin-6,12(7H)-dione,

1,17-bis(diphenylphosphino)-8,9,10,11-tetrahydro-, (17aR)- (9CI) (CA INDEX NAME)

RN 331768-67-3 CAPLUS

CN Dibenzo[b,d][1,6]dioxacyclotetradecin-6,13-dione, 1,18-bis(diphenylphosphino)-7,8,9,10,11,12-hexahydro-, (18aR)- (9CI) (CA INDEX NAME)

RN 331768-68-4 CAPLUS

CN Phosphine, [(17aR)-7,8,9,10,11,12-hexahydro-6H-dibenzo[b,d][1,6]dioxacyclotridecin-1,17-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 331768-69-5 CAPLUS

CN Dibenzo[b,d][1,6]dioxacyclotetradecin, 1,18-bis(diphenylphosphino)-6,7,8,9,10,11,12,13-octahydro-, (18aR)- (9CI) (CA INDEX NAME)

RN 331768-70-8 CAPLUS

CN Phosphine, [(19aR)-7,8,9,10,11,12,13,14-octahydro-6H-dibenzo[b,d][1,6]dioxacyclopentadecin-1,19-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 331768-71-9 CAPLUS

CN Phosphine, [(20aR)-6,7,8,9,10,11,12,13,14,15-decahydrodibenzo[b,d][1,6]dio xacyclohexadecin-1,20-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 331769-04-1 CAPLUS

CN 6H-Dibenzo[f,h][1,5]diazonine-6,8(7H)-dione, 1,13-bis(diphenylphosphino)-5,9-dihydro-, (13aR)- (9CI) (CA INDEX NAME)

RN 331769-05-2 CAPLUS

CN Dibenzo[b,d][1,6]diazecine-6,9-dione, 1,14-bis(diphenylphosphino)-5,7,8,10-tetrahydro-, (14aR)- (9CI) (CA INDEX NAME)

RN 331769-06-3 CAPLUS

CN 5H-Dibenzo[b,d][1,6]diazacycloundecine-6,10(7H,11H)-dione, 1,15-bis(diphenylphosphino)-8,9-dihydro-, (15aR)- (9CI) (CA INDEX NAME)

RN 331769-07-4 CAPLUS

CN Dibenzo[b,d][1,6]diazacyclododecine-6,11-dione, 1,16-bis(diphenylphosphino)-5,7,8,9,10,12-hexahydro-, (16aR)- (9CI) (CA INDEX NAME)

RN 331769-08-5 CAPLUS

CN 5H-Dibenzo[b,d][1,6]diazacyclotridecine-6,12(7H,13H)-dione, 1,17-bis(diphenylphosphino)-8,9,10,11-tetrahydro-, (17aR)- (9CI) (CA INDEX NAME)

$$Ph_2P$$
 $Ph_2P$ 
 $N$ 
 $H$ 

RN 331769-09-6 CAPLUS

CN Dibenzo[b,d][1,6]diazacyclotetradecine-6,13-dione, 1,18bis(diphenylphosphino)-5,7,8,9,10,11,12,14-octahydro-, (18aR)- (9CI) (CA INDEX NAME)

RN 331769-13-2 CAPLUS

CN 6H-Dibenzo[d,f][1,3]diazepin-6-one, 1,11-bis(diphenylphosphino)-5,7-dihydro-, (11aR)- (9CI) (CA INDEX NAME)

RN 331769-15-4 CAPLUS

CN Dibenzo[e,g][1,4]diazocine-6,7-dione, 1,12-bis(diphenylphosphino)-5,8-dihydro-, (12aR)- (9CI) (CA INDEX NAME)

RN 331769-16-5 CAPLUS

CN 5H-Dibenzo[d,f][1,3]diazepine, 1,11-bis(diphenylphosphino)-6,7-dihydro-, (11aR)- (9CI) (CA INDEX NAME)

RN 331769-17-6 CAPLUS

CN Dibenzo[e,g][1,4]diazocine, 1,12-bis(diphenylphosphino)-5,6,7,8-tetrahydro-, (12aR)- (9CI) (CA INDEX NAME)

RN 331769-18-7 CAPLUS

CN 5H-Dibenzo[f,h][1,5]diazonine, 1,13-bis(diphenylphosphino)-6,7,8,9-tetrahydro-, (13aR)- (9CI) (CA INDEX NAME)

RN 331769-19-8 CAPLUS

CN Dibenzo[b,d][1,6]diazacyclododecine, 1,16-bis(diphenylphosphino)-5,6,7,8,9,10,11,12-octahydro-, (16aR)- (9CI) (CA INDEX NAME)

RN 331769-20-1 CAPLUS

CN Phosphine, [(15aR)-6,7,8,9,10,11-hexahydro-5H-dibenzo[b,d][1,6]diazacycloundecine-1,15-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

331769-21-2 CAPLUS RN

5H-Dibenzo[b,d][1,6]diazacyclotridecine, 1,17-bis(diphenylphosphino)-CN 6,7,8,9,10,11,12,13-octahydro-, (17aR)- (9CI) (CA INDEX NAME)

RN331769-22-3 CAPLUS

CN Dibenzo[b,d][1,6]diazacyclotetradecine, 1,18-bis(diphenylphosphino)-5,6,7,8,9,10,11,12,13,14-decahydro-, (18aR)- (9CI) (CA INDEX NAME)

RN331776-92-2 CAPLUS

Dibenzo[b,d][1,6]diazecine, 1,14-bis(diphenylphosphino)-5,6,7,8,9,10-hexahydro-, (14aR)- (9CI) (CA INDEX NAME) CN

REFERENCE COUNT:

4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 2000:574233 CAPLUS

DOCUMENT NUMBER:

133:309942

TITLE:

Synthesis of Chiral Bisphosphines with Tunable Bite

Angles and Their Applications in Asymmetric

Hydrogenation of .beta.-Ketoesters

AUTHOR (S):

PUBLISHER:

LANGUAGE:

DOCUMENT TYPE:

CORPORATE SOURCE:

SOURCE:

Zhang, Zhaoguo; Qian, Hu; Longmire, James; Zhang, Xumu Department of Chemistry, The Pennsylvania State

University, University Park, PA, 16802, USA

Journal of Organic Chemistry (2000), 65(19), 6223-6226

CODEN: JOCEAH; ISSN: 0022-3263

American Chemical Society

Journal English

CASREACT 133:309942

OTHER SOURCE(S): GΙ

Ι

AΒ A series of chiral bisphosphines I (n = 1-6) with tunable dihedral angles were prepd. for the first time and used for Ru-catalyzed asym. hydrogenation of .beta.-ketoesters. Enantioselectivities with the Ru-I (n = 4) catalyst are comparable or better than those obsd. with Ru-BINAP and Ru-MeO-BIPHEP complexes, while enantioselectivities in asym. hydrogenation of .beta.-ketoesters are low with other catalysts e.g., Ru-I (n = 1, 6). The current study demonstrates the concept that changes in ligand dihedral angles indeed cause significant variations of enantioselectivity.

301847-87-0P 301847-88-1P 301847-89-2P IT 301847-90-5P 301847-91-6P 301847-92-7P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(synthesis of chiral bisphosphines with tunable bite angles and applications in asym. hydrogenation of beta-ketoesters)

301847-87-0 CAPLUS RN

Phosphine, (11aR)-dibenzo[d,f][1,3]dioxepin-1,11-diylbis[diphenyl- (9CI) CN (CA INDEX NAME)

301847-88-1 CAPLUS RN

CN Phosphine, [(12aR)-6,7-dihydrodibenzo[e,g][1,4]dioxocin-1,12diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-89-2 CAPLUS

CN Phosphine, [(13aR)-7,8-dihydro-6H-dibenzo[f,h][1,5]dioxonin-1,13-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-90-5 CAPLUS

CN Phosphine, [(14aR)-6,7,8,9-tetrahydrodibenzo[b,d][1,6]dioxecin-1,14-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-91-6 CAPLUS

CN Phosphine, [(15aR)-7,8,9,10-tetrahydro-6H-dibenzo[b,d][1,6]dioxacycloundec in-1,15-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

RN 301847-92-7 CAPLUS

CN Phosphine, [(16aR)-6,7,8,9,10,11-hexahydrodibenzo[b,d][1,6]dioxacyclododec in-1,16-diyl]bis[diphenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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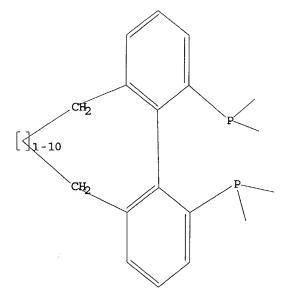
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> Uploading 09991261.str

L15 STRUCTURE UPLOADED

=> d L15 HAS NO ANSWERS L15 STR



G1 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s 115

SAMPLE SEARCH INITIATED 16:15:03 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 7 TO ITERATE

100.0% PROCESSED

7 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH

\*\*COMPLETE\*\*

PROJECTED ITERATIONS:

7 TO 298

PROJECTED ANSWERS:

0 TO (

L16

0 SEA SSS SAM L15

=> s 115 full

FULL SEARCH INITIATED 16:15:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 154 TO ITERATE

100.0% PROCESSED

154 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L17

0 SEA SSS FUL L15

=>

Uploading 09991261.str

L18

STRUCTURE UPLOADED

=> d

L18 HAS NO ANSWERS

L18

STR

G1 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s 118

SAMPLE SEARCH INITIATED 16:18:00 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -0 TO ITERATE

100.0% PROCESSED

0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH

\*\*COMPLETE\*\*

PROJECTED ITERATIONS:

O TO

PROJECTED ANSWERS:

0 TO

L19

0 SEA SSS SAM L18

=> s 118 full

FULL SEARCH INITIATED 16:18:10 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -0 TO ITERATE

100.0% PROCESSED

0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L20

0 SEA SSS FUL L18

Uploading 09991261.str

L21

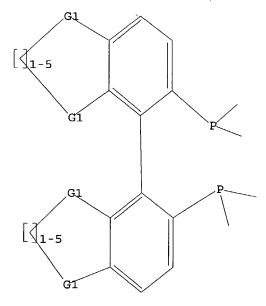
STRUCTURE UPLOADED

=> d

L21 HAS NO ANSWERS

L21

STR



G1 0, N

Structure attributes must be viewed using STN Express query preparation.

=> s 121

SAMPLE SEARCH INITIATED 16:19:27 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -2 TO ITERATE

100.0% PROCESSED

2 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:

ONLINE \*\*COMPLETE\*\*

BATCH

\*\*COMPLETE\*\* 124

PROJECTED ITERATIONS:

2 TO

PROJECTED ANSWERS:

1 TO

80

1 SEA SSS SAM L21

=> d scan

REGISTRY COPYRIGHT 2003 ACS L22 1 ANSWERS

Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[bis(4-chlorophenyl)-,

(+) - (9CI)

C38 H24 Cl4 O4 P2 MF

ALL ANSWERS HAVE BEEN SCANNED

Uploading 09991261.str

L23 STRUCTURE UPLOADED

=> d L23 HAS NO ANSWERS L23 STR

G1 O,N,S

Structure attributes must be viewed using STN Express query preparation.

=> s 123

SAMPLE SEARCH INITIATED 16:21:32 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2 TO 124
PROJECTED ANSWERS: 1 TO 80

L24 1 SEA SSS SAM L23

=> d

L24 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 210169-50-9 REGISTRY

CN Phosphine, [4,4'-bi-1,3-benzodioxole]-5,5'-diylbis[bis(4-chlorophenyl)-,

1 ANSWERS

(+)- (9CI) (CA INDEX NAME)

MF C38 H24 C14 O4 P2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 1 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> s 123 full FULL SEARCH INITIATED 16:21:57 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 56 TO ITERATE

100.0% PROCESSED 56 ITERATIONS

21 ANSWERS

SEARCH TIME: 00.00.01

L25 21 SEA SSS FUL L23

=> s l25 and s/els 5176232 S/ELS

L26 0 L25 AND S/ELS

=> s 125 and n/els 14477626 N/ELS

L27 0 L25 AND N/ELS

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ENTRY SESSION
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0.00
-10.42

FILE 'BEILSTEIN' ENTERED AT 16:23:42 ON 31 JAN 2003 COPYRIGHT (c) 2003 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein Chemiedaten & Software GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002

FILE COVERS 1779 TO 2001.
\*\*\* FILE CONTAINS 8,374,887 SUBSTANCES \*\*\*

- >>> For the revised summary sheet please see:
  http://info.cas.org/ONLINE/DBSS/beilsteinss.html <<</pre>
- >>> PLEASE NOTE: Reaction and substance documents are stored in
   different file segments. Use separate queries to search for
   reaction and substance data. When searching for bibliographic
   information you have the option to chose the file segment.
   (Use "/XXX.SUB" to search for a bibliographic term in
   substance documents. To restrict the search to reaction
   documents use "/XXX.RX".)
   For additional information see HELP RXS. <<<</pre>
- >>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

=> s 123 full FULL SEARCH INITIATED 16:23:47 FILE 'BEILSTEIN' FULL SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS SEARCH TIME: 00.00.04

=> d ide

### L28 ANSWER 1 OF 3 BEILSTEIN COPYRIGHT 2003 BEILSTEIN CDS MDL

Beilstein Records (BRN): 8893429 Chemical Name (CN): DTBM-SEGPHOS Autonom Name (AUN): 5,5'-bis-<br/>bis-(3,5-di-tert-butyl-4-methoxyphenyl)-phosphanyl>-<4,4'>bi<benzo<1,3>dioxolyl> Molec. Formula (MF): C74 H100 O8 P2 Molecular Weight (MW): 1179.55 Lawson Number (LN): 24014, 16730, 289 Compound Type (CTYPE): heterocyclic Constitution ID (CONSID): 7524026 8359415 Tautomer ID (TAUTID): Entry Date (DED): 2001/10/25 Update Date (DUPD): 2001/10/25

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

## Field Availability:

Code	Name	Occurrence			
BRN	Beilstein Records	1			
CN	Chemical Name	1			
AUN	Autonomname	1			
MF	Molecular Formula	1			
FW	Formular Weight	1			
LN	Lawson Number	3			
CTYPE	Compound Type	1			
CONSID	Constitution ID	1			
TAUTID	Tautomer ID	1			
ED	Entry Date	1			
UPD	Update Date	1			

### This substance also occurs in Reaction Documents:

Code	Name	Occurrence			
RX	Reaction Documents	1			
RXPRO	Substance is Reaction Product	1			

#### => d his

(FILE 'HOME' ENTERED AT 15:40:00 ON 31 JAN 2003)

```
FILE 'REGISTRY' ENTERED AT 15:40:06 ON 31 JAN 2003
L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 1 S L2
L4 21 S L2 FULL
```

FILE 'CAPLUS' ENTERED AT 16:05:27 ON 31 JAN 2003 L5 10 S L4

```
0 S L4 FULL
L6
L7
              0 S L1 FULL
L8
              3 S L2 FULL
     FILE 'REGISTRY' ENTERED AT 16:10:56 ON 31 JAN 2003
L9
               STRUCTURE UPLOADED
L10
              4 S L9
             56 S L9 FULL
L11
             53 S L11 NOT SI/ELS
L12
L13
             50 S L12 NOT OL
     FILE 'CAPLUS' ENTERED AT 16:12:41 ON 31 JAN 2003
L14
              6 S L13
     FILE 'REGISTRY' ENTERED AT 16:14:44 ON 31 JAN 2003
L15
               STRUCTURE UPLOADED
L16
              0 S L15
L17
              0 S L15 FULL
L18
               STRUCTURE UPLOADED
L19
             0 S L18
L20
             0 S L18 FULL
L21
              STRUCTURE UPLOADED
L22
             1 S L21
L23
               STRUCTURE UPLOADED
L24
             1 S L23
L25
             21 S L23 FULL
L26
             0 S L25 AND S/ELS
L27
             0 S L25 AND N/ELS
     FILE 'BEILSTEIN' ENTERED AT 16:23:42 ON 31 JAN 2003
L28
             3 S L23 FULL
=>
Executing the logoff script...
=> LOG H
COST IN U.S. DOLLARS
                                                 SINCE FILE
                                                               TOTAL
                                                      ENTRY SESSION
FULL ESTIMATED COST
                                                       8.55
                                                              926.26
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                 SINCE FILE
                                                               TOTAL
                                                     ENTRY
                                                              SESSION
CA SUBSCRIBER PRICE
                                                       0.00
                                                              -10.42
SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 16:25:40 ON 31 JAN 2003
Welcome to STN International! Enter x:x
LOGINID:ssspta1204jxv
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2
```

\* \* \* \* \* \* \* \* \* Welcome to STN International

FILE 'BEILSTEIN' ENTERED AT 16:06:59 ON 31 JAN 2003

```
Web Page URLs for STN Seminar Schedule - N. America
NEWS 1
NEWS 2
         Apr 08
                 "Ask CAS" for self-help around the clock
NEWS 3
         Apr 09
                 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS
         Apr 09
                 ZDB will be removed from STN
NEWS 5
         Apr 19
                 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6
         Apr 22
                 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
     7
                 BIOSIS Gene Names now available in TOXCENTER
NEWS
         Apr 22
NEWS 8
         Apr 22
                 Federal Research in Progress (FEDRIP) now available
NEWS 9
         Jun 03
                 New e-mail delivery for search results now available
NEWS 10
         Jun 10
                 MEDLINE Reload
NEWS 11
         Jun 10
                 PCTFULL has been reloaded
NEWS 12
                 FOREGE no longer contains STANDARDS file segment
         Jul 02
NEWS 13
         Jul 22
                 USAN to be reloaded July 28, 2002;
                 saved answer sets no longer valid
NEWS 14
         Jul 29
                 Enhanced polymer searching in REGISTRY
NEWS 15
         Jul 30
                 NETFIRST to be removed from STN
NEWS 16
         Aug 08
                 CANCERLIT reload
NEWS 17
         Aug 08
                 PHARMAMarketLetter (PHARMAML) - new on STN
NEWS 18
         Aug 08
                 NTIS has been reloaded and enhanced
NEWS 19
         Aug 19
                 Aquatic Toxicity Information Retrieval (AQUIRE)
                 now available on STN
NEWS 20
         Aug 19
                 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21
        Aug 19
                 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22
         Aug 26
                 Sequence searching in REGISTRY enhanced
NEWS 23
         Sep 03
                 JAPIO has been reloaded and enhanced
NEWS 24
         Sep 16
                 Experimental properties added to the REGISTRY file
NEWS 25
        Sep 16
                CA Section Thesaurus available in CAPLUS and CA
NEWS 26 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 27 Oct 21 EVENTLINE has been reloaded
NEWS 28 Oct 24 BEILSTEIN adds new search fields
NEWS 29 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 30 Oct 25 MEDLINE SDI run of October 8, 2002
NEWS 31 Nov 18 DKILIT has been renamed APOLLIT
NEWS 32 Nov 25 More calculated properties added to REGISTRY
NEWS 33 Dec 02 TIBKAT will be removed from STN
NEWS 34 Dec 04 CSA files on STN
NEWS 35 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 36 Dec 17
                TOXCENTER enhanced with additional content
NEWS 37 Dec 17 Adis Clinical Trials Insight now available on STN
NEWS 38 Dec 30 ISMEC no longer available
NEWS 39 Jan 13 Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 40 Jan 21 NUTRACEUT offering one free connect hour in February 2003
NEWS 41 Jan 21 PHARMAML offering one free connect hour in February 2003
NEWS 42 Jan 29
                Simultaneous left and right truncation added to COMPENDEX,
                 ENERGY, INSPEC
NEWS EXPRESS January 6 CURRENT WINDOWS VERSION IS V6.01a,
              CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
NEWS INTER
              General Internet Information
NEWS LOGIN
              Welcome Banner and News Items
NEWS PHONE
             Direct Dial and Telecommunication Network Access to STN
NEWS WWW
             CAS World Wide Web Site (general information)
```

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 18:26:20 ON 31 JAN 2003

=> file stnguide
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'STNGUIDE' ENTERED AT 18:26:26 ON 31 JAN 2003 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Jan 24, 2003 (20030124/UP).

=> d his

(FILE 'HOME' ENTERED AT 18:26:20 ON 31 JAN 2003)

FILE 'STNGUIDE' ENTERED AT 18:26:26 ON 31 JAN 2003

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.12 0.33

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 18:27:28 ON 31 JAN 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 JAN 2003 HIGHEST RN 483965-49-7 DICTIONARY FILE UPDATES: 30 JAN 2003 HIGHEST RN 483965-49-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

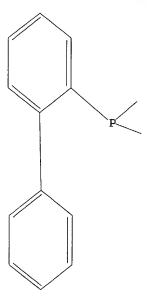
Uploading 09991261.str

L1 STRUCTURE UPLOADED

=> s ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):end SEARCH ENDED BY USER

### L1 HAS NO ANSWERS

L1



G1 0,N,S

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 18:27:54 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 166 TO ITERATE

100.0% PROCESSED

166 ITERATIONS

31 ANSWERS

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2547 TO 4093

PROJECTED ANSWERS: 286 TO

L231 SEA SSS SAM L1

=> d scan

L231 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Phosphine, (1,1-dimethylethyl) phenyl [2'-[(trimethylsilyl) oxy] [1,1'-

biphenyl]-2-yl]- (9CI)

MF C25 H31 O P Si